Robert S. Kerr Environmental Research Center
Center for Subsurface Modeling Support (CSMoS)

Ground-Water and Vadose Zone Models / Manuals
July 2000

Ordering Instructions

Preferred Method

Download models and manuals via:

Homepage: http://www.epa.gov/ada/kerrcenter.html
Anonymous FTP: ftp.epa.gov/pub/ada/models

Note:
Manuals are in **PDF** format. Users can download the free **Adobe Acrobat Reader** program (link provided) and install on hard drive. Users can then open **PDF** files within the program to read, navigate through, and print documents.

Alternate Method
- Request specific model(s) on company letterhead (specify DOS or WIN when appropriate).
- Models and manuals will be distributed on diskettes **(Adobe Acrobat Reader included)**.
- Include appropriate number of required diskettes. Please send **NEW (no labels attached)**, pre-formatted, 3.5", high density diskettes (Summary Table provided on page 5).
  NOTE: USED diskettes will not be accepted.
- All models/manuals are free of charge.

Send requests to: Robert S. Kerr Environmental Research Center
                          Center for Subsurface Modeling Support (CSMoS)
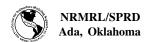   P.O. Box 1198
                          919 Kerr Research Drive
                          Ada, OK   74821-1198
                          580-436-8586
                          580-436-8718 (FAX)
                          Co-Directors: Dr. David S. Burden (580-436-8606)
                                            Dr. David G. Jewett (580-436-8560)

For further information regarding distribution, please call
580-436-8756 or email kinsey.jason@epa.gov.

2DFATMIC - Source Code (Version 1.0 - August 1997) - Available on Internet Homepage Only

Application:	Simulates subsurface flow, transport, and fate of contaminants which are undergoing chemical and/or biological transformations. The model is applicable to transient conditions in both saturated and unsaturated zones.
Processes:	The flow module is a Galerkin finite element solution of Richard's equation. The transport module is a hybrid Lagrangian-Eulerian approach with an adapted zooming and peak capturing algorithm.
Miscellaneous:	This model can almost eliminate spurious oscillation, numerical dispersion, and peak clipping due to advective transport.
Notice:	For support on this model contact - Professor G.T. Yeh (814)863-2931

3DFATMIC- Source Code (Version 1.0 - August 1997) - Available on Internet Homepage Only

Application:	Simulates subsurface flow, transport, and fate of contaminants which are undergoing chemical and/or biological transformations. The model is applicable to transient conditions in both saturated and unsaturated zones.
Processes:	The flow module is a Galerkin finite element solution of Richard's equation. The transport module is a hybrid Lagrangian-Eulerian approach with an adapted zooming and peak capturing algorithm.
Miscellaneous:	This model can almost eliminate spurious oscillation, numerical dispersion, and peak clipping due to advective transport.
Notice:	For support on this model contact - Professor G.T. Yeh (814)863-2931

BIOCHLOR (Version 1. - June 2000)

Application:	BIOCHLOR is a screening model that simulates remediation by natural attenuation of dissolved solvents at chlorinated solvent release sites. BIOCHLOR can be used to simulate solute transport without decay and solute transport with biodegredation modeled as a sequential first-order process within 1 or 2 different reaction zones.
Processes:	The program is based on the 1-D Domenico analytical solute transport model and includes 1-D advection, 3-D dispersion, linear adsorption and biotransformation via reductive dechlorination. Reductive dechlorination is assumed to occur under anaerobic conditions and solvent degradation is assumed to follow a sequential first-order decay process.
Miscellaneous:	The BIOCHLOR Program is written as an Excel Spreadsheet and therefore requires Microsoft Excel to run. The program includes a Natural Attenuation Screening Protocol scoring system to help the user determine the potential for reductive dechlorination from site data.

BIOPLUME II (Version 1.1 - October 1989)

Application:	Two-dimensional contaminant transport under the influence of oxygen limited biodegradation.
Processes:	Advection, dispersion, sorption, biodegradation (aerobic and anaerobic) and reaeration.
Miscellaneous:	Model is based on the 2-D solute transport code, USGS-MOC.

BIOPLUME III (Version 1.0 - September 1997)

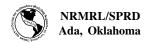|	
Application:	Two-dimensional contaminant transport under the influence of oxygen, nitrate, iron, sulfate, and methanogenic biodegradation.
Processes:	Advection, dispersion, sorption, first order decay, biodegradation through instantaneous, first order, zero order, or Monod kinetics.
Miscellaneous:	Model is based on 2-D solute transport code, USGS-MOC but has an integrated, Windows based, graphical user interface for seamless preprocessing and output review. Hydrocarbon source and each active electron acceptor are simulated as separate plumes.

BIOSCREEN (Version 1.4 - July 1997)

Application: Three-dimensional contaminant transport for dissolved phase hydrocarbons in saturated zone under the influences of oxygen, nitrate, iron, sulfate, and methane limited biodegradation.
Processes: Advection, dispersion, adsorption, first-order decay, and instantaneous reactions under aerobic and anaerobic conditions.
Miscellaneous: An easy-to-use screening tool which is based on the Domenico analytical solute transport model.

CHEMFLO (Version 1.30 - August 1989)

Application: Simulation of 1-D water and chemical movement in vadose zone.
Processes: Advection, dispersion, first-order decay and linear sorption.
Miscellaneous: Numerical solution, handles a variety of boundary conditions.

GEOEAS (Version 1.2.1 - April 1991) - Available on Internet Homepage Only

Application: Geostatistical analysis of spatially correlated data.
Components: Basic statistics, scatter plots/linear and nonlinear estimation (kriging).

GEOPACK (Version 1.0.e - January 1990)

Application: Geostatistical analysis of spatially correlated data.
Components: Basic statistics, variography, linear and nonlinear estimation (kriging).

HSSM (DOS Version 1.10 - April 1994) or (Windows Version 1.20a - September 1997) - Specify DOS or WIN Version

Application: Simulates flow of the LNAPL phase and transport of a chemical constituent of the LNAPL from the surface to the water table; radial spreading of the LNAPL phase at the water table; and dissolution and aquifer transport of the chemical constituent.
Processes: One-dimensional in the vadose zone, radial in the capillary fringe, two-dimensional vertically averaged analytical solution of the advection-dispersion equation in the saturated zone.
Miscellaneous: Model is based on the KOPT, OILENS and TSGPLUME models. This model is also available in Spanish.

A Manual of Instructional Problems for the U.S.G.S. MODFLOW Model (February 1993)

Application: Instructional manual (study guide) for the USGS MODFLOW Model.
Components: A series of twenty problem sets that illustrate by example the use of MODFLOW including modeling principles, input/output specifics, available options, rules of thumb, and common modeling mistakes, etc.

MOFAT (Version 2.0a - May 1991)

Application: Two-dimensional flow and transport of three fluid phases: water, nonaqueous phase liquid, and gas.
Processes: Advection, dispersion, diffusion, sorption, decay, mass transfer.
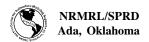Miscellaneous: Finite-element, numerous parameters required.

MT3D (Version 1.11 - January 1992)

Application: Three-dimensional contaminant transport in the saturated zone.
Processes: Advection, dispersion, nonlinear sorption, first-order irreversible decay, and biodegradation.
Miscellaneous: Numerical solution, uses hybrid method of characteristics, particle tracking, handles a variety of discretization schemes and boundary conditions, includes MODFLOW program.

NAPL Simulator (Version 1.0 October 1997) - Available on Internet Homepage Only

Application:	Simulation of the contamination of soils and aquifers which results from the release of organic liquids commonly referred to as Non-Aqueous Phase Liquids (NAPL).
Processes:	The simulator is applicable to three interrelated zones: a vadose zone which is in contact with the atmosphere, a capillary zone, and a water-table aquifer zone. Three mobile phases are accommodated: water, NAPL, and gas. The 3-phase k-S-P sub-model accommodates capillary and fluid entrapment hysteresis. NAPL dissolution and volatilization are accounted for through rate-limited mass transfer sub-models.
Miscellaneous:	The numerical solution is based on a Hermite collocation finite element discretization. The simulator provides an accurate solution of a coupled set of nonlinear partial differential equations that are generated by combining fundamental balance equations with constitutive thermodynamic relationships.
Notice:	For support on this model contact - Joseph Guarnaccia (732) 914-2516

OASIS (Macintosh - Version 2.1 - May 1994)

Application:	A decision support system for contaminant transport modeling.
Components:	A hydrogeologic database, two chemical databases, Bioplume II and a few other simple hydrogeologic models.

PESTAN (Version 4.0)

Application:	Vadose zone modeling of the transport of organic (pesticide) contaminants.
Processes:	Advection, dispersion, first-order decay and linear sorption.
Miscellaneous:	Screening model, few parameters required.

RETC (Version 1.1 - November 1994)

Application:	Estimates soil-water retention curve, unsaturated hydraulic conductivity or soil model parameters.
Processes:	Uses the parametric equations of Brooks-Corey, van Genuchten and the pore-size distribution models of Maulem and Burdine.
Miscellaneous:	Analytical model, requires relatively few parameters.

RITZ (Version 2.12 - January 1988)

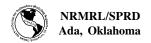|	
Application:	Vadose zone modeling of the transport of contaminants associated with oily wastes.
Processes:	Water movement, volatilization, degradation, sorption and leaching.
Miscellaneous:	Analytical model, requires relatively few parameters.

STF (Version 2.0 - June 1991)

Application:	Database providing information concerning the behavior of organic and a few inorganic chemicals in the soil environment.
Components:	Degradation, transformation, toxicity, bioaccumulation and partitioning.
Miscellaneous:	RITZ and VIP models included.

UTCHEM (Version 6.1 - February 1999)

Application: Originally a three-dimensional finite difference model for multiphase flow, transport and chemical flooding, the UTCHEM code has been modified to transform it into a general purpose NAPL simulator. Appropriate physical, chemical and biological process models have been incorporated into the simulator to create a 3D multiphase multicomponent model capable of simulating the fate and transport of NAPL's in the saturated and unsaturated zones of aquifers. The model can be used to simulate the actual field operation of remediation activities such as surfactant remediation or bioremediation as well as laboratory experiments with large-scale aquifer models.

Processes: UTCHEM is capable of modeling transient and steady-state three-dimensional flow and mass transport in the groundwater (saturated) and vadose (unsaturated) zones of aquifers. Physical, chemical and biological process models important in describing the fate and transport of NAPL's in contaminated aquifers have been incorporated into the simulator. These include multiple organic NAPL phases; the dissolution and/or mobilization of NAPL's by non-dilute remedial fluids; chemical and microbiological transformations; and changes in fluid properties as a site is remediated. The model allows for non-equilibrium interphase mass transfer; sorption; geochemical reactions; and the temperature dependence of pertinent chemical and physical properties. It can simulate the flow and transport of remedial fluids whose density, temperature and viscosity are variable, including surfactants, co-solvents and other enhancement agents. The biodegradation model includes inhibition, sequential use of electron acceptors, and co-metabolism and can be used to model a very general class of bioremediation processes.

Miscellaneous: Biodegradation capabilities have been added to describe the transformation of organic contaminants from NAPL sources and can accommodate multiple substrates, electron acceptors and biological species. A new multiphase capillary-pressure and relative-permeability function has been added to allow the use of either Brooks-Corey or Van Genuchten capillary pressure functions. New organic and tracer components have been added as well as additional water tracer components and gas phase tracers. The number of oil/water tracers has been expanded to allow any number of tracer components. The geochemical option has been extended to allow the modeling of any solid or aqueous species. UTCHEM uses a solution scheme analogous to the Implicit Pressure Explicit Saturation (IMPES) routine where the pressure is solved for implicitly but concentrations instead of saturations are solved in a flash routine. An energy balance equation includes heat flow between the reservoir and the over- and under- burden rocks.

Notice: For support on this model contact - Dr. Gary Pope, Department of Petroleum Engineering, University of Texas, Austin, TX.

VLEACH (Version 2.2a - June 1996)

Application: Simulation of 1-D water and chemical movement in vadose zone.
Processes: Advection, sorption, vapor-phase diffusion, three-phase equilibration.
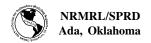Miscellaneous: Numerical solution, screening model.

WhAEM (Version 1.00b - August 1996)

Application: Delineates capture zones and isochrones of groundwater residence time for the purpose of "wellhead protection."
Processes: Steady-state, homogeneous, isotropic, advection and dispersion.
Miscellaneous: Consists of two independent executables: GAEP (Geographic Analytic Element Preprocessor) and

CZAEM (Capture Zone   Analytic Element Model).

WhAEM 2000 (Version 1.0.3 - June 2000)

Application: Delineates capture zones and isochrones of ground-water residence time for the purpose of "source water area delineation" and "wellhead protection".
Processes: Steady-state, homogeneous, isotropic, advection.
Miscellaneous: Full 32-bit graphical user interface for Windows (95,98,NT). On-line help and tutorial. Working with WhAEM2000 document demonstrates modeling practice for Vincennes, Indiana, case study.
Notice: For support on this model contact - Stephen R. Kraemer; Phone: 706-355-8340; Fax: 706-355-8302; E-mail: kraemer.stephen@epa.gov
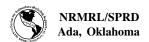
WHPA (Version 2.2 - September 1993)

Application: Simulates capture zones for pumping wells.
Processes: Steady-state, horizontal flow.
Miscellaneous: Particle-tracking with analytical, semi-analytical, numerical modules.

Model Distribution by Diskette

Summary Table

MODEL NAME	MODEL DISKS	MANUAL DISKS
BIOCHLOR	1	1
BIOPLUME II	1	1
BIOPLUME III	2	HARD COPY
BIOSCREEN	2	1
CHEMFLO	1	1
GEOPACK	2	1
HSSM (DOS OR WIN)	2	2
MFINSTRU MANUAL*	0	5
MOFAT	1	2
MT3D	2	2
OASIS (Macintosh)	6	HARD COPY
PESTAN	1	1
RETC	1	2
RITZ	1	1
STF	2	1
VLEACH	1	1
WhAEM	1	2
WHPA	2	3

* A Manual of Instructional Problems for the U.S.G.S. MODFLOW Model

Note: Add 1 diskette for Adobe Acrobat Reader per total request.

Example 1:
Requested Geopack - 4 disks
2 disks - model
1 disk - manual
1 disk - Reader

Example 2:
Requested Geopack and Pestan - 6 disks
2 disks - model Geopack
1 disk - model Pestan
1 disk - manual Geopack
1 disk - manual Pestan
1 disk - Reader